Nuclear Energy University Programs

NEAMS Reactor IPSC:
Nuclear Reactor Performance and Safety Analysis

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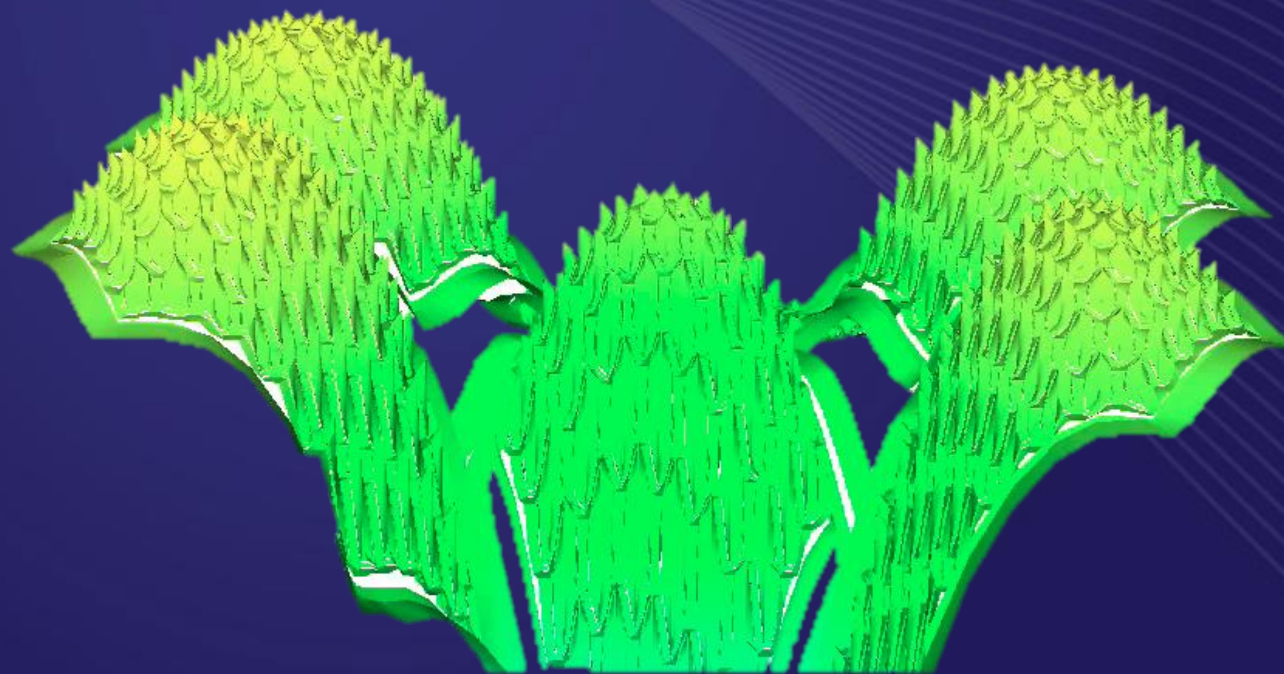


Overview

- **Relationship between NEET and NEAMS**
- **Overview of NEAMS**
- **Reactor Integrated Performance and Safety Codes**
  - Nuclear Reactor Performance and Safety Analysis
- **FY12 Reactor IPSC Scope**
- **FY12 NEUP Scope to Address Research Needs**
- **Expectations and Deliverables**

Funding and Programmatic Overview

- **Nuclear Energy Enabling Technologies (NEET)**
  - Crosscutting Technologies
    - Modeling and Simulation
- **Nuclear Energy Advanced Modeling and Simulation (NEAMS)**
  - Integrated Performance and Safety Codes (IPSC)
    - Reactor IPSC
  - Supporting Elements

- **In FY 2012 NEAMS will be supported by NEET**

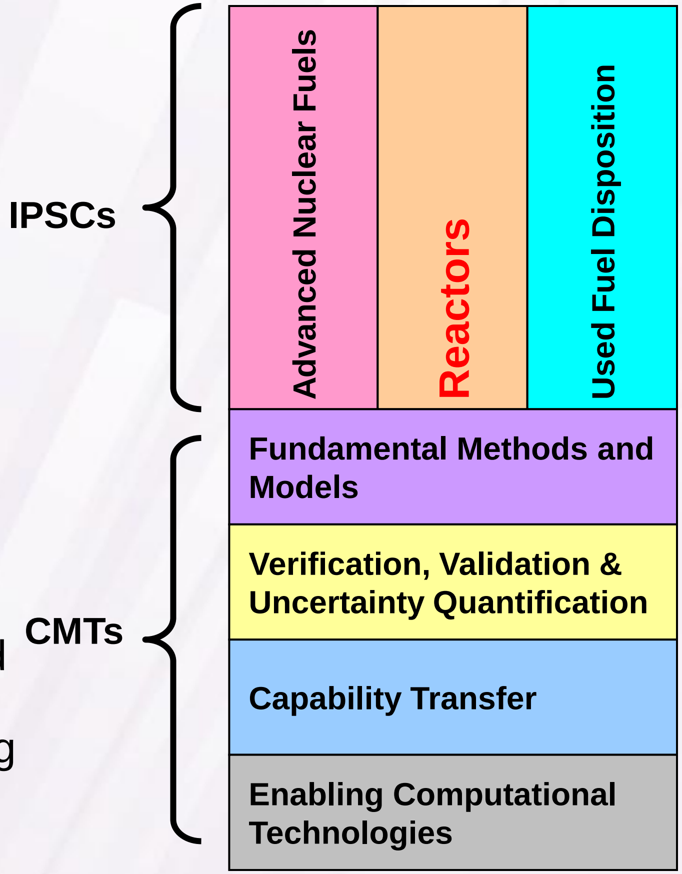
Purpose of NEAMS

Produce and deliver computational tools to designers and analysts that *predict behavior* in relevant operating regimes, particularly beyond the test base.

NEAMS Program Elements

- **Integrated Performance and Safety Codes**
  - Continuum level codes that will **predict** the **performance** and **safety** of nuclear energy systems technologies
  - Attributes include 3D, science based physics, high resolution, integrated systems
  - Long-term development horizon (~10 years)
  - Codes with verification, validation and error uncertainty quantification
  - Using interoperability frameworks and modern software development techniques and tools

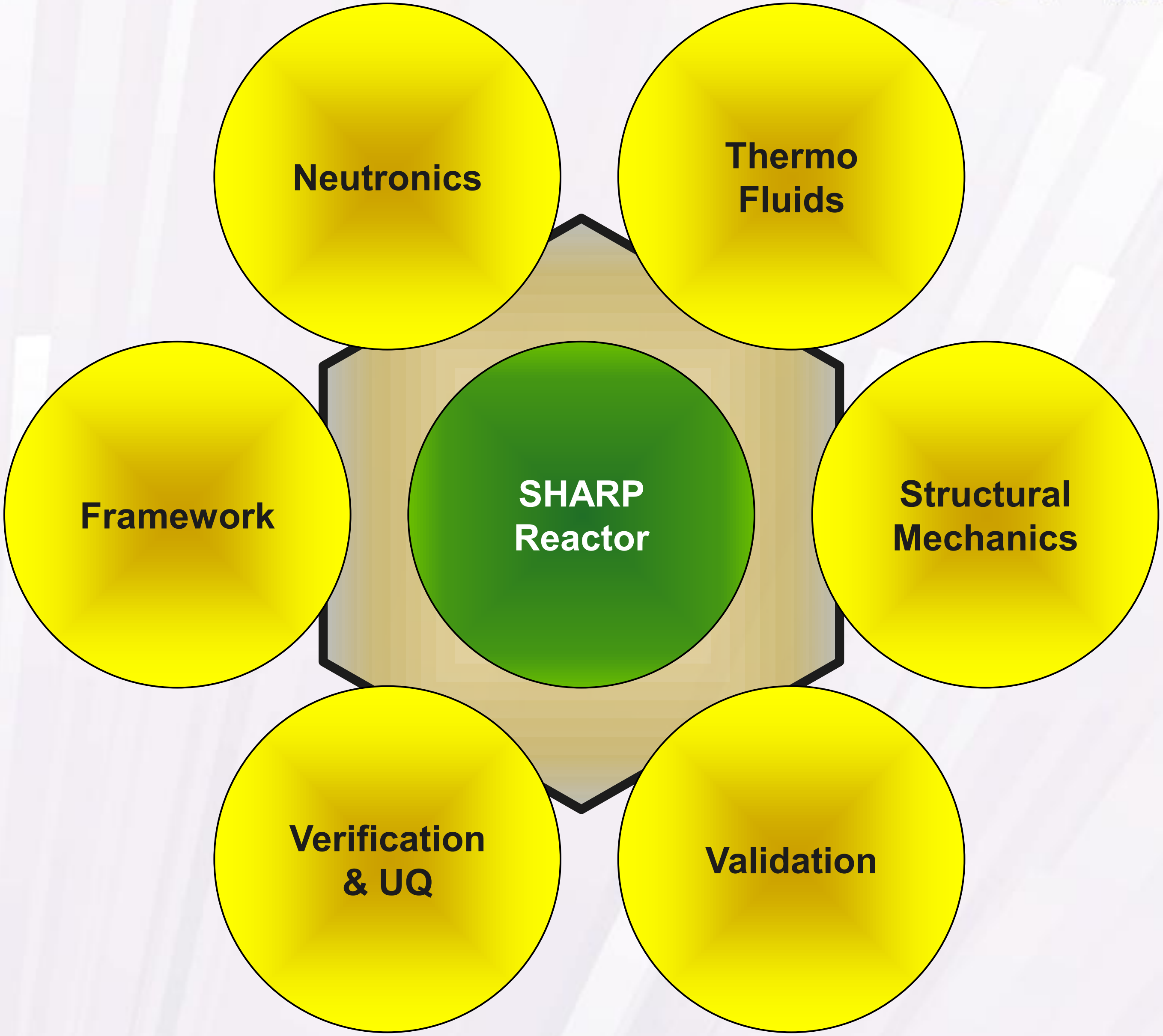
- **Crosscutting Methods and Tools**
  - Develop crosscutting (i.e. more than one IPSC) required capabilities
  - Provide a single NEAMS point of contact for crosscutting requirements (e.g. experimental data, computer technologies)
  - Smaller, more diverse teams to include laboratories, universities and industries.
  - “Tool Development” with shorter timelines



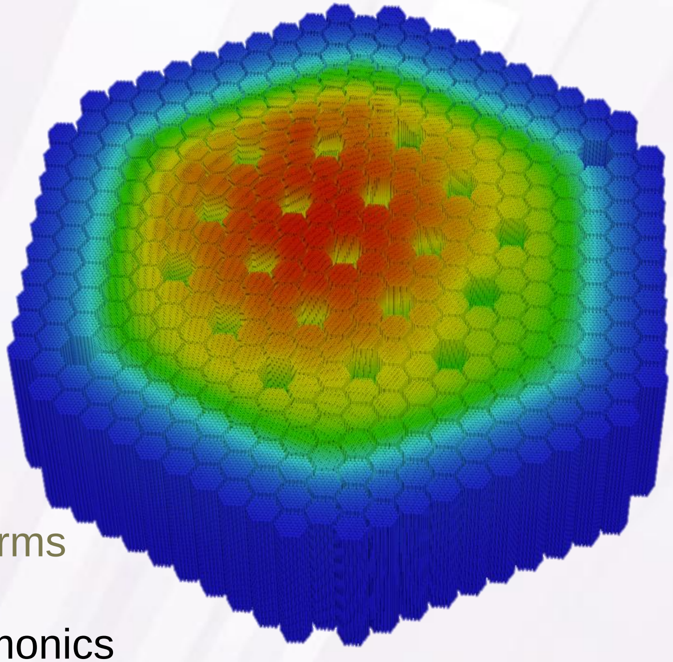
Reactor IPSC Goals and Strategy

- **Apply modern, high-performance computing techniques to nuclear reactor modeling**
  - Use advanced simulation tools to improve safety, reduce cost, explore advanced designs
  - Provide local data needed to enable predictive fuel performance simulations
  - Understand and reduce uncertainty of computational models
- **Strategy**
  - Focus funding on reactor agnostic components to remain responsive to customer needs
  - Adopt multi-scale strategy to enable application to problems relevant to industry using a wide range of platforms
  - Utilize modular architecture to enable component-wise use by most advanced users or integrated user interface driven application by less advanced users.
  - Develop collaborations with customers to define near term applications/demonstrations
- **Customers**
  - Advanced Reactor Concepts
  - Next Generation Nuclear Plant
  - Light Water Reactor Sustainability
  - Small Modular Reactors

SHARP Reactor

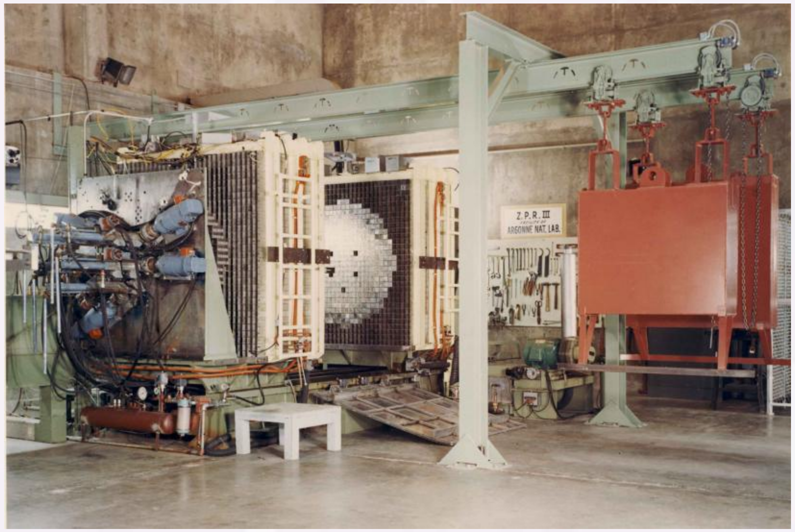

Neutronics
Thermo Fluids
Framework
SHARP Reactor
Structural Mechanics
Verification & UQ
Validation

Neutronics (Proteus)

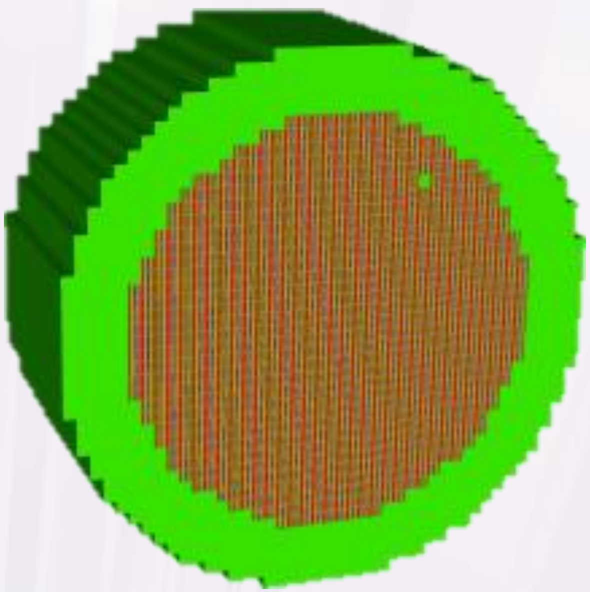


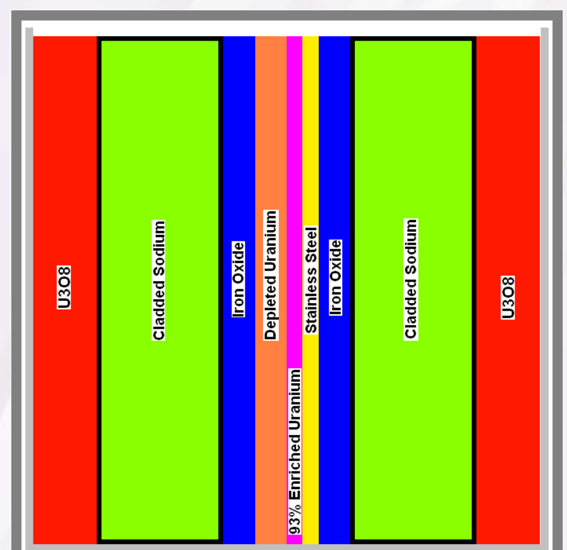
- **MC^2-3 module**
  - Provides high resolution cross-section libraries for fast spectrum applications
- **UNIC transport solver modules**
  - MOC-FE provides 3-D & 2-D MOC
    - targeting problems with minimal homogenization
  - SN2ND provides 1st and 2nd Order Discrete Ordinates
    - demonstrated from desktop to petascale platforms
    - prefer to homogenize pin cells
  - PN2ND provide 1st and 2nd Order Spherical Harmonics
    - prefer to homogenize assembly internals
  - NODAL provides a diffusion theory based structured geometry solver
    - fast running, highly scalable full core simulator
- **MOCARV simulation module**
  - Integrates 2-D MOC representations of radial planes with Sn Transport in axial direction
- **Simulation modules to support reactor kinetic and fuel cycle analysis using the UNIC transport solver modules are in preliminary stages of development**

Neutronics Validation



- **ZPR6 Assembly 6A**
  - Well-documented critical experiment
- **Recent Developments:**
  - $2 \times 10^6 \rightarrow +50 \times 10^6$
  - 20 M vertices, 100 angles, 33 groups, ~45 min on full Cray XT5 (~130B DOF)

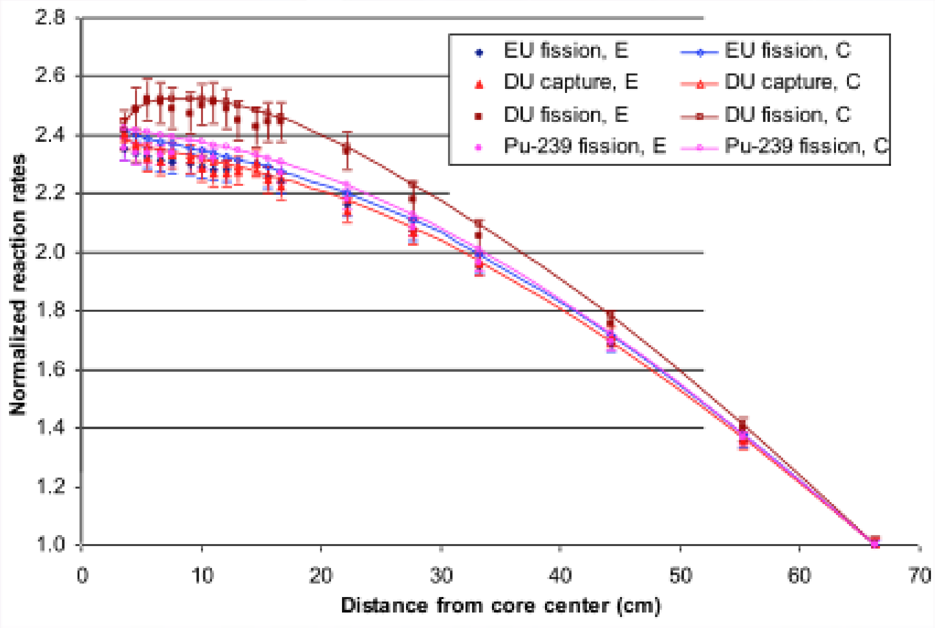


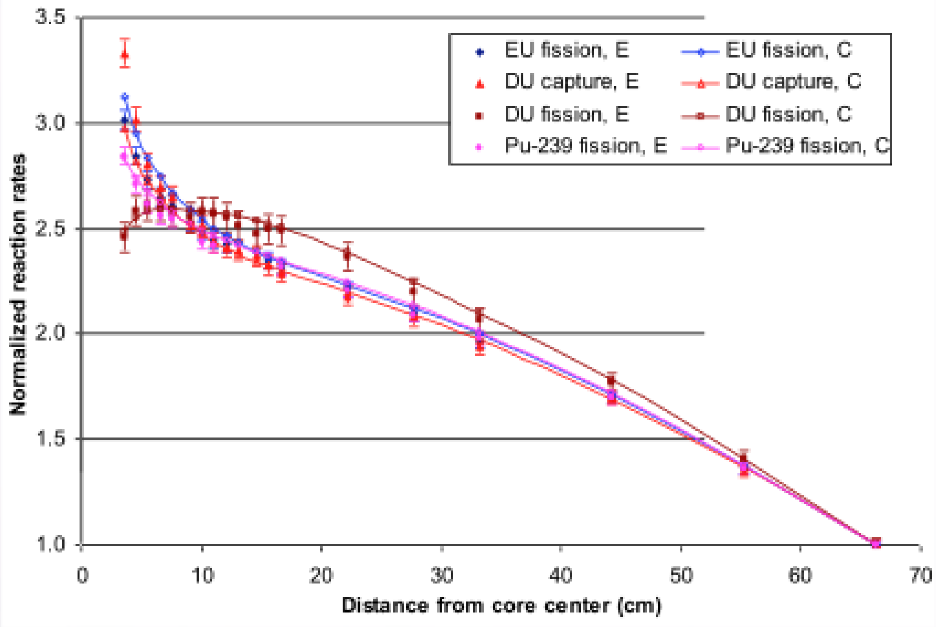


Exact Geometry

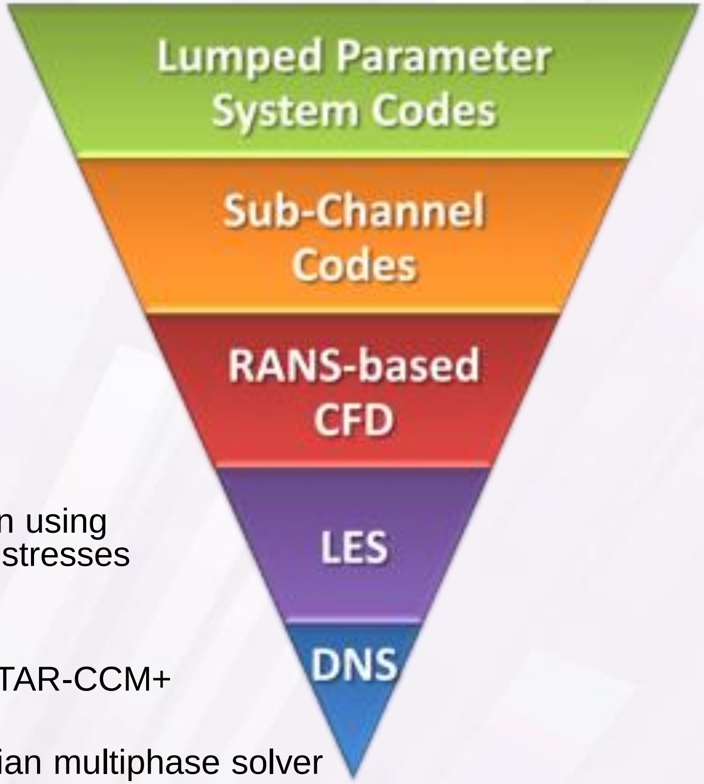
ZPR6-7 Foil Measurements

- 230 group L5T5 with P3 scattering kernel were performed using SN2ND
- Existing VARIANT code could not obtain a similar solution
- Results shown are for fission in the EU foils and capture in the DU foils for the two BeO modified loadings
- Results for loadings 104 and 120 using foil cross sections from MC^2-3 were equivalent in accuracy to that using MCNP based foil cross sections
- Additional Studies are ongoing on how to improve MC^2-3 performance and accuracy





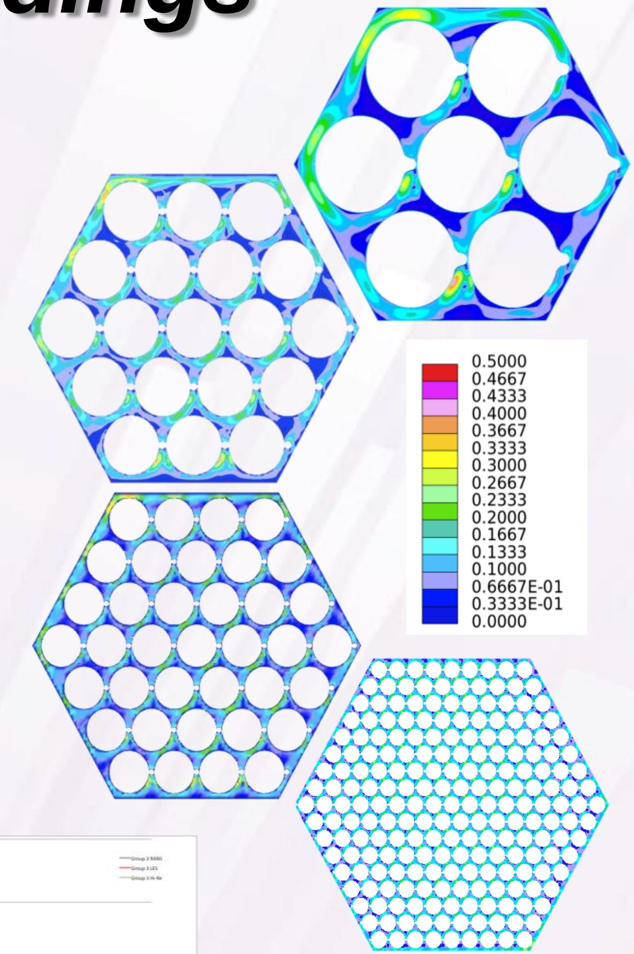
Thermal Hydraulics

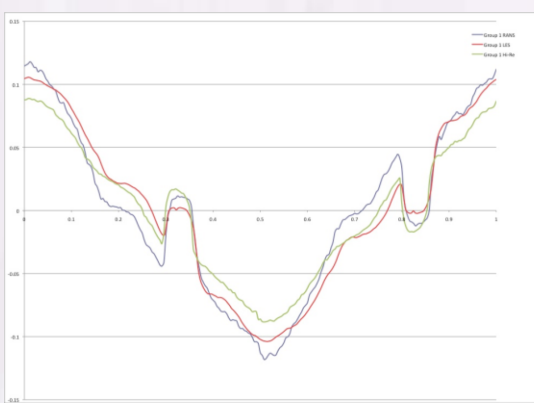


- **Nek5000 DNS/LES module**
  - Highly-scalable, high-order spectral element CFD
  - Direct Numerical Simulation
    - solves for stress tensor directly
    - limited to small regions because very high resolution mesh is needed
  - Large Eddy Simulation
    - uses spectral filtering or sub-grid model for smallest turbulence length scales
    - applicable to component analysis
- **Nek5000 URANS module**
  - Solves Unsteady Reynolds Averaged Navier Stokes equation using two to six equation closure models to approximate turbulent stresses
  - Applicable to large regions
- **STAR-CCM+**
  - Provides access to steady and unsteady RANS solvers of STAR-CCM+
  - Applicable to large regions, up to full core
  - Provides access to STAR-CCM+ steady state eulerian-eulerian multiphase solver
- **SHARP-IF module**
  - Intermediate fidelity simulation toolset using momentum sources to mimic effects of geometric details
  - Applicable to full core +
- **SAS11 modules**
  - Lumped parameter representation of T/H and Structural Mechanics applicable to full system
  - Provides continued access to existing SFR fuel performance models

Thermal Hydraulics Findings

- **Flow field evolves significantly from 7 to 217 pin assemblies**
  - Reduced importance of bulk swirling and increased complexity of flow field with increasing pin count
  - Fundamental change in flow behavior between 19- and 37-pin assemblies
    - Important because most experiments have been completed using 19 pins
    - Explains observations in small number of experimental pressure drop data sets for large bundles

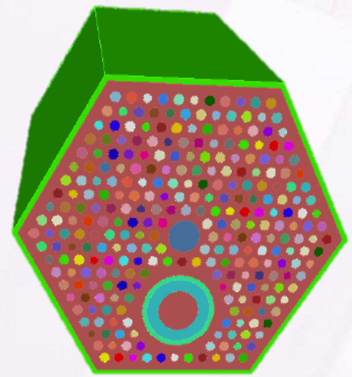


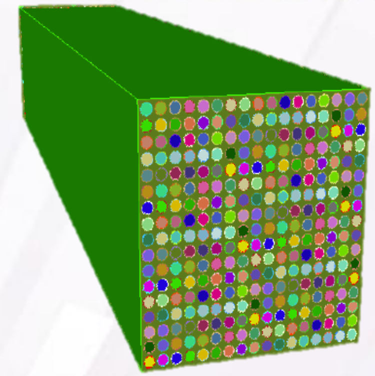


Framework and Meshing

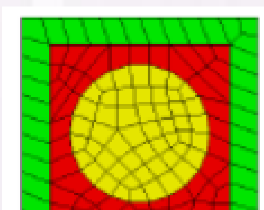
- **MOAB module**
  - Highly scalable data management for mesh based simulations
  - Currently integrated into UNIC, Nek5000, Star-CCM+ and DIABLO
- **MB Coupler module**
  - Scalable parallel solution transfer between meshes of different types
- **MeshKit Modules**
  - MeshKit Generation Library
    - Provides consistent API access mesh generation functionalities in MeshKit or other libraries
    - Includes RGG reactor geometry/meshing tool
  - CGM Geometry Library
    - Library for CAD and other geometry types
    - Includes interface to Open.CASCADE, an open-source library for geometry
    - compatible with (and can import models from) CUBIT's CGM
  - Lasso relations library
    - Allows associate of mesh to geometry without requiring software dependency between mesh and geometry libraries

Meshing

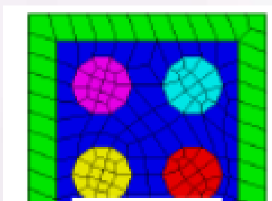




- **MeshKit's RGG (Reactor Geometry Generator) has two components:**
  - AssyGen: Assembly geometry and meshes based on text input. Supports rectangular and hexagonal assemblies

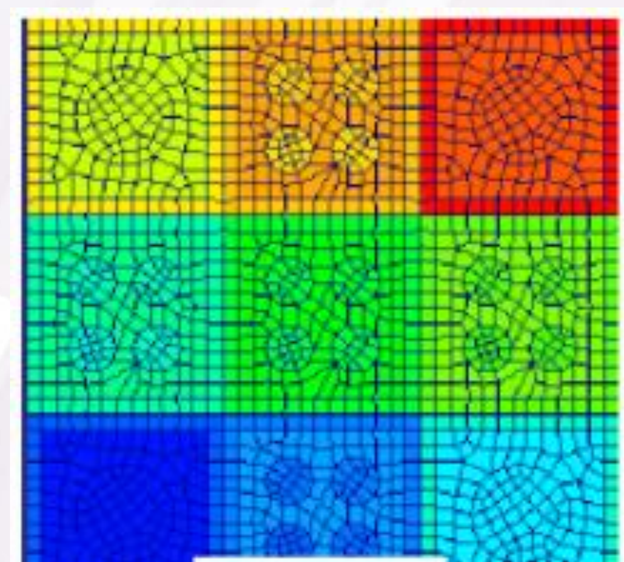


Assembly Mesh 2



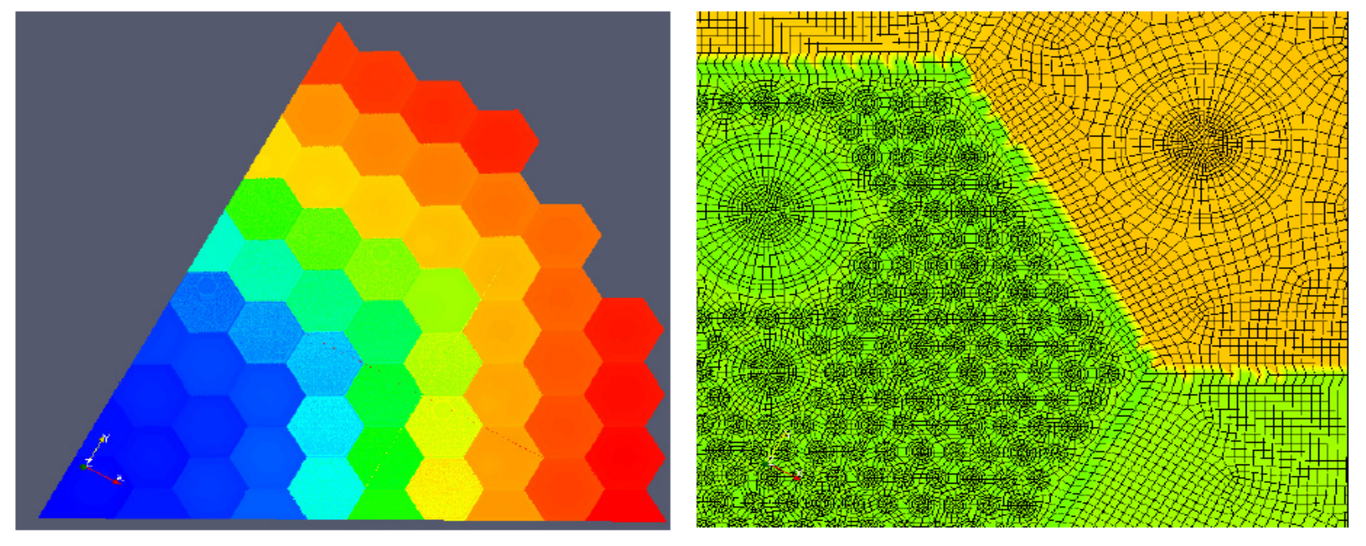
Assembly Mesh

  - Coregen: Core geometry and meshes by copy, move and merge operations.



Core mesh

Meshing



- **1/6th of a VHTR core (12M hexes)**
  - Assembly geometry: 4 min
  - Assembly meshing: 4 min
  - Copy/move/merge assemblies to form the reactor core: 23 min

Planned FY12 Workscope

- **Neutronics**
  - Finalize QA work on intermediate-fidelity neutronics
  - Wrap up remaining work on MC^2-3
  - Update MOCFE to handle non-conformal spatial meshes
  - Support data structures for conventional sub-group cross-section treatment for thermal reactors.
  - Update MOCARV (reduced vector space solution algorithm with parallel solve) and perform verification
  - Prepare documentation for SN2ND
  - Develop additional verification benchmarks

Planned FY12 Workscope

- **Thermal Hydraulics**
  - Continue QA work for Nek5000
  - Prepare validation benchmark simulation for 2012 OECD/NEA MATiS benchmark
  - Continue developments and validation for Nek5000-based uRANS solver
  - Extend IF treatment to whole-assembly models
  - Assess whole-assembly flow and temperature distributions for transient conditions.
  - Develop dynamic multiscale averaging techniques for turbulence simulations.

Planned FY12 Workscope

- **Framework and Meshing**
  - Continue integration of UNIC, Nek, and Diablo into SHARP framework.
  - Improve performance and flexibility of solution transfer.
  - Implement surface field coupling
  - Implement boundary-layer tool for inserting post-meshing boundary conditions
  - Establish MeshKit/MOAB/CGM user workshop and documentation

Planned FY12 Workscope

- **Systems and Safety**
  - Review potential compatibility between R7 and SHARP
  - Formulate case studies for cross-fidelity comparisons between reduced- and high-fidelity simulations
  - Define algorithmic requirements for reduced-fidelity model caliabration
  - Update code documentation for SAS11
  - Establish automated verification and regression testing

Planned FY12 Workscope

- **Structural and Fuel Mechanics**
  - Complete Diablo connection to the MOAB API
  - Demonstrate thermal-mechanical coupling
  - Establish representative assembly geometry with operational power and flow history for fuel mechanics simulations
  - Perform simulations using AMP to predict assembly distortion due to power/flow history.
- **Uncertainty Quantification ($200k)**
  - Perform uncertainty analysis for Nek-5000 2D validation examples
  - Continue developments of automatic differentiation techniques applied to SAS11

Challenges

- Multi-Resolution Scaling and Multi-Physics Coupling
- Thermal-Hydraulics
- Safety Analyses
- Meshing
- Visualization

Reactor IPSC Research Needs

- **Multi-Resolution Scaling and Multi-Physics Coupling**
  - Upscaling methods that enable reduced order modeling of long term transients and fuel cycle performance.
  - Multi-scale integration methods to enable development of virtual reactor simulations using multiple levels of resolution to represent a single physics.
  - Modular structural codes to understand all aspects of pressure boundary integrity (piping, vessels, steam generators, nozzles etc.).

Reactor IPSC Research Needs

- **Thermal-Hydraulics**
  - Methods to perform sensitivity studies to evaluate variability and/or flow dominance regimes during the initiating phases of natural convection cooling.
  - Predictive methods for simulation of two-phase boiling and/or flashing flows in complex geometry.
  - Water coolant chemistry models to support simulation of steam generating fouling and in-core applications.
  - Development of a coolant properties code library that contains highly-detailed correlations and uncertainty quantification data on coolant properties in liquid, vapor, and supercritical phases (e.g. provide a reference for benchmark and validation purposes).

Reactor IPSC Research Needs

- **Safety Analyses**
  - Multi-scale integration methods to enable development of virtual reactor simulations using multiple levels of resolution to represent different physics (e.g., neutronics, fluid dynamics, heat transfer, etc.)
  - Methods to perform probabilistic safety assessment of component or system performance weighted over a broad spectrum of anticipated component or inherent feature failure conditions.
  - Development of a coolant properties code library that contains highly-detailed correlations and uncertainty quantification data on coolant properties in liquid, vapor, and supercritical phases (e.g. provide a reference for benchmark and validation purposes).

Reactor IPSC Research Needs

- **Meshing**
  - Efficient, scalable, high-fidelity mesh generation methods to provide accurate descriptions of realistic nuclear reactor component geometries
- **Visualization**
  - Expanded visualization techniques to assess system-wide coupling impacts

Expectations and Deliverables

- **Mission-driven expectations**
  - 20% relevance
  - 80% technical
- **Deliverables clearly tied to Reactor IPSC needs and identified in proposals**
  - Specific
  - Measurable
  - Achievable
  - Realistic
  - Time-bound
- **Performance feedback**